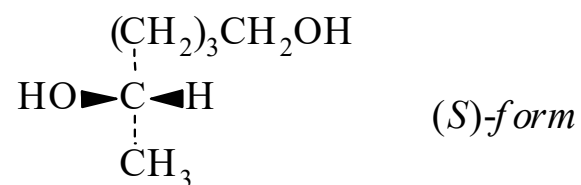




>>Entry Name: 1,5-Hexanediol, 9CI

ENTRY UNDER REVIEW



CAS Registry Number: 928-40-5

Related CAS Registry Numbers(s): 71401-68-8

Extra CAS Registry Numbers(s): 26762-52-7

Molecular Formula: C₆H₁₄O₂

Molecular Weight: 118.175

Accurate Mass: 118.09938

Percentage Composition: C 60.98%; H 11.94%; O 27.08%

Aldrich: 19818-8

>>Variant: (S)-form

CAS Registry Number: 109784-17-0

Molecular Formula: C₆H₁₄O₂

Molecular Weight: 118.175

Accurate Mass: 118.09938

Percentage Composition: C 60.98%; H 11.94%; O 27.08%

Biological Source: Obt. from Brefeldin A [CJZ31-J](#)

Physical Description: Oil

Optical Rotation: $[\alpha]_{\text{D}}^{20} +8$ (c, 0.55 in MeOH)

>>Derivative: Bis-4-nitrobenzoyl

Molecular Formula: C₂₀H₂₀N₂O₈

Molecular Weight: 416.387

Percentage Composition: C 57.69%; H 4.84%; N 6.73%; O 30.74%

Physical Description: Cryst. (CH₂Cl₂/pentane)

Melting Point: Mp 107-108°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +43$ (c, 0.43 in CHCl₃)

>>Variant: (±)-form

Molecular Formula: C₆H₁₄O₂

Molecular Weight: 118.175

Accurate Mass: 118.09938

Percentage Composition: C 60.98%; H 11.94%; O 27.08%

Use/Importance: Uses include antiperspirant and food additive

Boiling Point: Bp₁₇ 140-141°. Bp_{0.5} 89-91°

>>Derivative: Bis-4-nitrobenzoyl

Melting Point: Mp 89-90°

References:

- Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 134C, (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 202C, (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 196A, (*ir*)
Perkin, W.H., *J.C.S.*, 1887, **51**, 702, (*synth*)
Sigg, H.P., *Helv. Chim. Acta*, 1964, **47**, 1401, (*abs config, ir, pmr*)
Voitsekhovskoya, A.L. *et al.*, *CA*, 1967, **66**, 55320x, (*synth*)
Moore, B.P. *et al.*, *Aust. J. Chem.*, 1976, **29**, 1365, (*synth*)
Davies, S.G. *et al.*, *J.C.S. Perkin I*, 1996, 2467, (*synth*)